



Aalborg Universitet

**AALBORG UNIVERSITY**  
DENMARK

## **Hydrophilic-to-Hydrophobic Transition in Glassy Silica is Driven by the Atomic Topology of its Surface**

Yu, Yingtian; Krishnan, N. M. Anoop; Smedskjær, Morten Matstrup; Sant, Gaurav; Bauchy, Mathieu

*Publication date:*  
2018

[Link to publication from Aalborg University](#)

*Citation for published version (APA):*

Yu, Y., Krishnan, N. M. A., Smedskjær, M. M., Sant, G., & Bauchy, M. (2018). *Hydrophilic-to-Hydrophobic Transition in Glassy Silica is Driven by the Atomic Topology of its Surface*. Abstract from 2018 Glass and Optical Materials Division Annual Meeting, San Antonio, Texas, United States.

### **General rights**

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal -

### **Take down policy**

If you believe that this document breaches copyright please contact us at [vbn@aub.aau.dk](mailto:vbn@aub.aau.dk) providing details, and we will remove access to the work immediately and investigate your claim.

**(GOMD-S1-141-2018) Hydrophilic-to-Hydrophobic Transition in Glassy Silica is Driven by the Atomic Topology of its Surface**

Y. Yu<sup>1</sup>; N. Krishnan<sup>2</sup>; M. M. Smedskjaer<sup>3</sup>; G. Sant<sup>\*1</sup>; M. Bauchy<sup>1</sup>

*1. University of California, Los Angeles, USA 2. Indian Institute of Technology Delhi, India 3. Aalborg University, Denmark*

The surface reactivity and hydrophilicity of silicate materials are key properties for various industrial applications. However, the structural origin of their affinity for water remains unclear. Here, based on reactive molecular dynamics simulations of a series of glassy silica surfaces annealed at various temperatures and subsequently exposed to water, we show that silica exhibits a hydrophilic-to-hydrophobic transition driven by its silanol surface density. By applying topological constraint theory, we show that the surface reactivity and hydrophilic/hydrophobic character of silica are controlled by the atomic topology of its surface. This suggests that novel silicate materials with tailored reactivity and hydrophilicity could be developed through the topological nanoengineering of their surface.